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Abstract

In this note new diagonal-implicit Runge-Kutta methods for semi-explicit PDAEs of index 2 are presented. These solvers are stiffly accurate, of order 3 for the ODE-variables and of order 2 for the algebraic variables. They have three and four internal stages and automatic steplength control by the help of embedding is possible. The methods with four internal stages have a stiffly accurate embedded method of order 2 for all variables. The methods are applied on the incompressible Navier-Stokes equations and compared with other DIRK-methods.

1 Introduction

The incompressible Navier-Stokes equations describe the motion of an incompressible fluid and are given (in dimensionless form) by

$$\begin{aligned} \mathbf{u}_t - \epsilon^{-1}\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p &= \mathbf{f} && \text{in } (0,T]\times\Omega, \\ \nabla\cdot\mathbf{u} &= 0 && \text{in } [0,T]\times\Omega, \\ \mathbf{u} &= \mathbf{g} && \text{on } [0,T]\times\partial\Omega, \\ \mathbf{u}(0,\cdot) &= \mathbf{u}_0 && \text{in } \Omega, \\ \int_\Omega p\,d\mathbf{x} &= 0 && \text{in } [0,T]. \end{aligned} \tag{1}$$

In (1) $\mathbf{u}$ denotes the velocity, $\mathbf{u}_0$ the initial velocity and p the pressure. The term $\mathbf{f}$ represents body forces and $\mathbf{g}$ the given Dirichlet boundary data. For the pressure p no boundary conditions are needed since we require that $p \in L_0^2(\Omega)$. Let $[0,T]$ be a given time interval and $\Omega \subset \mathbb{R}^d$, $d \in \{2,3\}$, a domain. The Navier-Stokes equations posses as parameter the Reynolds number ϵ. Depending on ϵ, different flow regimes are described with (1). If ϵ is sufficiently small and the data in (1) do not depend on the time, $(\mathbf{u},p)$ represent a stationary flow field. For larger ϵ, the flow is time-dependent and laminar; and for large ϵ, the flow becomes turbulent. The accurate and fast solution of the Navier-Stokes equations is the core of many numerical simulations.

In a first step we semi-discretise the incompressible Navier-Stokes-equations (1) in space with a finite element method. For simplicity of presentation, we consider only the case of homogeneous Dirichlet boundary conditions. Writing (1) component-wise

$$\dot{u}_1 - \epsilon^{-1}\Delta u_1 + u_1\partial_x u_1 + u_2\partial_y u_1 + \partial_x p = f_1, \tag{2}$$
$$\dot{u}_2 - \epsilon^{-1}\Delta u_2 + u_1\partial_x u_2 + u_2\partial_y u_2 + \partial_y p = f_2, \tag{3}$$
$$\partial_x u_1 + \partial_y u_2 = 0, \tag{4}$$

with $\mathbf{u} = (u_1, u_2)^T$, multiplying (2)-(4) by test functions $\mathbf{v} = (v_1, v_2)^T \in V := (H_0^1(\Omega))^2$, $q \in Q = L_0^2(\Omega)$, integrating over Ω and applying integration by parts, we obtain the following weak problem: Find $(\mathbf{u}, p) \in L^2(0,T;V) \times L^2(0,T;Q)$ with $\mathbf{u} = (u_1, u_2)^T$ such that a.e. in $(0,T)$

$$\begin{aligned}
(\dot{u}_1, v_1) + \epsilon^{-1}(\nabla u_1, \nabla v_1) + (u_1\partial_x u_1 + u_2\partial_y u_1, v_1) + (\partial_x p, v_1) &= (f_1, v_1),\\
(\dot{u}_2, v_2) + \epsilon^{-1}(\nabla u_2, \nabla v_2) + (u_1\partial_x u_2 + u_2\partial_y u_2, v_2) + (\partial_y p, v_2) &= (f_2, v_2),\\
(u_1, \partial_x q) + (u_2, \partial_y q) &= 0
\end{aligned}$$

holds for all $(\mathbf{v}, q) \in V \times Q$. The finite element method approximates the solution of the weak problem in some finite dimensional subspaces $V^h \subset V$ and $Q^h \subset Q$. Let $V^h = W^h \times W^h$, $\{\varphi_1, \ldots, \varphi_{N_u}\}$ be a basis of W^h and $\{\psi_1, \ldots, \psi_{N_p}\}$ be a basis of Q^h. The following matrices and vectors are defined:

$$\begin{aligned}
(M)_{ij} &= (\varphi_j, \varphi_i), && i,j = 1,\ldots,N_u,\\
(A_{11}(\mathbf{u}))_{ij} &= \epsilon^{-1}(\nabla\varphi_j, \nabla\varphi_i)\\
&\quad + (u_1\partial_x\varphi_j + u_2\partial_y\varphi_j, \varphi_i), && i,j = 1,\ldots,N_u,\\
(A_{22}(\mathbf{u}))_{ij} &= (A_{11})_{ij}, && i,j = 1,\ldots,N_u,\\
(B_1)_{ij} &= (\partial_x\psi_j, \varphi_i), && i = 1,\ldots,N_u, j = 1,\ldots,N_p,\\
(B_2)_{ij} &= (\partial_y\psi_j, \varphi_i), && i = 1,\ldots,N_u, j = 1,\ldots,N_p,\\
(f_k)_i &= (f_k, \varphi_i), && i = 1,\ldots,N_u, \quad k = 1,2.
\end{aligned}$$

With these settings, we get the so-called MOL-DAE

$$\begin{pmatrix} M & 0 & 0\\ 0 & M & 0\\ 0 & 0 & 0 \end{pmatrix}\begin{pmatrix} \dot{u}_1\\ \dot{u}_2\\ \dot{p} \end{pmatrix} = \begin{pmatrix} f_1\\ f_2\\ 0 \end{pmatrix} - \begin{pmatrix} A_{11}(\mathbf{u}) & 0 & B_1\\ 0 & A_{22}(\mathbf{u}) & B_2\\ B_1^T & B_2^T & 0 \end{pmatrix}\begin{pmatrix} u_1\\ u_2\\ p \end{pmatrix}$$

or shorter

$$\begin{pmatrix} M & 0\\ 0 & 0 \end{pmatrix}\begin{pmatrix} \dot{\mathbf{u}}\\ \dot{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f}\\ 0 \end{pmatrix} - \begin{pmatrix} A(\mathbf{u}) & B\\ B^T & 0 \end{pmatrix}\begin{pmatrix} \mathbf{u}\\ p \end{pmatrix} \tag{5}$$

Equation (5) is a differential-algebraic equation (DAE) of index 2 (see [3]).

Let us now consider the time-discretisation of (5) as it is described in [15, 19] with some modifications considered in [25]. Let τ_n be the current time step from t_n to t_{n+1}, i.e. $\tau_n = t_{n+1} - t_n$. We denote quantities at time level t_m by a subscript m. To describe the time stepping scheme for the incompressible Navier-Stokes equations (1), a general time step of the form

$$\begin{aligned} (M + \theta\tau_n A(\mathbf{u}_{m+1}))\mathbf{u}_{m+1} + \tau_n B p_{m+1} & \\ = \; & (M - (1-\theta)\tau_n A(\mathbf{u}_m))\mathbf{u}_m - (1-\theta)\tau_n B p_m \qquad (6) \\ & +(1-\theta)\tau_n \mathbf{f}_m + \theta\tau_n \mathbf{f}_k, \qquad (7) \\ B^\top \mathbf{u}_{m+1} \; = \; & 0, \end{aligned}$$

with the parameter θ can be introduced. The time step (6) allows the implementation of a number of time stepping schemes by one single formula and the choice between the schemes by setting the parameter θ.

Three well known one-step θ-schemes are obtained by appropriate choices of this parameter, see Table 1.

Table 1: One-step θ-schemes

	θ	t_m	t_{m+1}	τ_m
forward Euler scheme	0	t_n	t_{n+1}	τ_n
backward Euler scheme	1	t_n	t_{n+1}	τ_n
Crank-Nicolson scheme (CN)	1/2	t_n	t_{n+1}	τ_n

The fractional-step θ-scheme, [4, 8], is obtained by three suitable steps of form (6). We want to present only one variant of this scheme. Let

$$\theta = 1 - \frac{\sqrt{2}}{2}, \quad \tilde\theta = 1 - 2\theta, \quad \alpha = \frac{\tilde\theta}{1-\theta}, \quad \beta = 1 - \alpha. \qquad (8)$$

One variant (we call it FS in the following) is presented in Table 2.

Table 2: A variant of the fractional-step θ-scheme

	θ	t_m	t_{m+1}	τ_m
FS	$\alpha\theta$	t_n	$t_n + \theta\tau_n$	$\theta\tau_n$
	$\beta\tilde\theta$	$t_n + \theta\tau_n$	$t_{n+1} - \theta\tau_n$	$\tilde\theta\tau_n$
	$\alpha\theta$	$t_{n+1} - \theta\tau_n$	t_{n+1}	$\theta\tau_n$

There are a number of investigations of the time discretizations introduced above applied to the Navier-Stokes equations, see Gresho and Sani [9, Section

3.16] or Emmrich [7, Section 4.1] for a survey of the present state of art. The Crank-Nicolson scheme was studied by Temam [29], Heywood and Rannacher [12] and Bause [2] for the already spatially discretized Navier-Stokes equations (with a finite element method). One can prove, under a number of assumptions on the smoothness of the data, that the error between the time discrete and the time-continuous finite element velocity in $L^\infty(0,T;L^2(\Omega))$ behaves like $(\tau)^2$ for the equidistant time step τ. The fractional-step θ-scheme was investigated analytically by Klouček and Rys [20] and Müller-Urbaniak [22]. A second order error estimate similar to the Crank-Nicolson scheme was proved in [22].

The Crank-Nicolson and the fractional-step θ-scheme are widely used in the numerical solution of the incompressible Navier-Stokes equations, [30, 16]. The Crank-Nicolson scheme is A-stable whereas the fractional-step θ-scheme is even strongly A-stable. That means, the Crank-Nicolson scheme may lead to numerical oscillations in problems with rough initial data or boundary conditions. These oscillations are damped out only if sufficiently small time steps are used. Compared to the fractional-step θ-scheme, a smaller time step might be necessary for the Crank-Nicolson scheme to ensure robustness.

From [25] we know that we can rewrite the θ-schemes as diagonally implicit Runge-Kutta methods, so-called DIRK methods. In [26] the fractional-step-θ scheme with an embedded method is introduced. It is possible to solve ODE by the help of the fractional-step-θ scheme and automatic time steplength control using the so-called embedding technique. Since the fractional-step-θ-method has some disadvantages, i.e. order reduction for the Prothero-Robinson problem (see [25, 26]) we suggest some new DIRK methods in this note. These schemes should have three or four internal stages, should be at least strongly A-stable and have convergence order 2 for the example of Prothero and Robinson (see [23]).

The paper is structured as follows. In Section 2 we introduce Runge-Kutta-methods and take a look on convergence results. New methods are designed in Section 3 and 4. Finally we present some numerical experiments solving the incompressible Navier-Stokes equations.

2 Runge-Kutta methods for implicit ODEs

In the following we consider the ordinary differential equation (ODE)

$$M\dot{\mathbf{u}} = \mathbf{F}(t,\mathbf{u}), \qquad \mathbf{u}(0) = \mathbf{u}_0, \tag{9}$$

where M is the so called mass-matrix which is regular. Next we define a Runge-Kutta method (see [11, 28]).

Definition 2.1 *Let $s \in \mathbb{N}$. The one-step-method*

$$M\mathbf{k}_i = \mathbf{F}(t_m + c_i\tau, \mathbf{u}_m + \tau \sum_{j=1}^{s} a_{ij}\mathbf{k}_j) \tag{10}$$

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \tau \sum_{i=1}^{s} b_i\mathbf{k}_i \tag{11}$$

is called s-stage Runge-Kutta method (RK method). The numbers a_{ij}, b_i and c_i are the coefficients of the method.

An RK method can be described by the help of the so-called Butcher-table which was originally proposed by Butcher [5]

$$\begin{array}{c|ccc} c_1 & a_{11} & \dots & a_{1s} \\ c_2 & a_{21} & \dots & a_{2s} \\ \vdots & \vdots & & \vdots \\ c_s & a_{s1} & \dots & a_{ss} \\ \hline & b_1 & \dots & b_s \end{array} = \begin{array}{c|c} \mathbf{c} & A \\ \hline & \mathbf{b}^\top \end{array}.$$

The value s is called number of stages. The vector $\mathbf{c}$ includes the grid points of the time-discretisation and $\mathbf{b}$ is vector with some weights. The coefficients a_{ij}, b_i and c_i should be choosen in such a way that some order conditions are satisfied to obtain a sufficient consistency order. In Table 3 we present the order conditions up to order 3 (see for example [11, 28]). It is possible to construct Runge-Kutta

Table 3: Order conditions for Runge-Kutta methods up to order 3

Nr.	order	order condition
1	1	$\sum b_i = 1$
2	2	$\sum b_i c_i = 1/2$
3	3	$\sum b_i c_i^2 = 1/3$
4	3	$\sum b_i a_{ij} c_j = 1/6$

methods by the help of so-called simplifying conditions which were orginally introduced by Butcher [5].

$$\begin{aligned}
B(p): \quad & \sum_{i=1}^{s} b_i c_i^{k-1} &&= 1/k && k = 1,\ldots,p,\\
C(q): \quad & \sum_{j=1}^{s} a_{ij} c_j^{k-1} &&= c_i^k/k && i = 1,\ldots,s, k = 1,\ldots,q,\\
D(r): \quad & \sum_{i=1}^{s} b_i c_i^{k-1} a_{ij} &&= b_j(1-c_j^k)/k && j = 1,\ldots,s, k = 1,\ldots,r.
\end{aligned}$$

The simplifying condition $C(q)$ can be written in the form $A\mathbf{c}^{k-1} = \mathbf{c}^k/k$, where $\mathbf{c}^k = (c_1^k,\ldots,c_s^k)^\top$.

The stability function $R_0(z)$ of our Runge-Kutta method (10), (11) is given by

$$R_0(z) = 1 + z\mathbf{b}^\top (I - zA)^{-1}\mathbf{e}, \quad \mathbf{e} = (1,\ldots,1)^\top \in \mathbb{R}^s. \tag{12}$$

Next we introduce some stability concepts.

Definition 2.2 *A Runge-Kutta method* (10), (11) *is called A-stable, if*

$$R_0(z) \le 1, \qquad \forall z \in \mathbb{C}^-.$$

An A-stable Runge-Kutta method is called strongly A-stable, if

$$\lim_{Re\, z\to -\infty} |R_0(z)| < 1.$$

Moreover we call an A-stable Runge-Kutta method L-stable, if

$$\lim_{Re\, z\to -\infty} |R_0(z)| = 0.$$

A Runge-Kutta method satisfying

$$a_{si} = b_i \quad \text{and} \quad c_s = 1$$

is called *stiffly accurate*.

It is well-known that Runge-Kutta methods have order reduction if they are applied on stiff ODEs or differential algebraic equations (DAEs). More informations about that interesting topic can be found in the books of [28] and [11] and the literature cited in both books or in [25].

Definition 2.3 *Consider a Runge-Kutta method with consistency order p. Moreover the method should satisfy the simplifying condition $C(q)$. Then the minimum of p and q is called stage order of the Runge-Kutta method.*

Solving a stiff ODE with the help of a Runge-Kutta method the convergence order may drop down from p to q, if $p > q$ (see [11]).

Throughout this note we consider only Runge-Kutta methods with $s \geq 3$ and coefficients satisfying the hypotheses

$$
\begin{aligned}
&(H1) : a_{ij} = 0, \quad i < j, i, j \in \{1, \ldots, s\}, \\
&(H2) : a_{11} = 0, \\
&(H3) : a_{ii} \neq 0, \quad i \in \{2, \ldots, s\}, \\
&(H4) : b_i = a_{si}, \quad i \in \{1, \ldots, s\}
\end{aligned}
$$

Runge-Kutta methods satisfying $(H1)$ are called diagonal-implicit Runge-Kutta methods (DIRK methods). These methods are discussed in several papers and books [28, 11].

Lemma 1 *A Runge-Kutta method satisfying $a_{11} \neq 0$ and $(H1)$ has at most stage order $q = 1$.*

Proof Condition $C(2)$ implies for $i = 1$

$$a_{11}c_1 = a_{11}^2 = a_{11}/2.$$

It follows $a_{11} = 0$, but this is contraction to our assumption $a_{11} \neq 0$. $\square$

Lemma 2 *A Runge-Kutta method satisfying $(H1)$, $(H2)$ and $(H3)$ can have at least stage order $q = 2$.*

Proof The expression $C(2)$ implies

$$a_{21}c_1 + a_{22}c_2 = a_{22}(a_{21} + a_{22}) = (a_{21} + a_{22})^2/2.$$

It follows $a_{21} = a_{22}$. Next we consider the condition $C(3)$, i.e. $A\mathbf{c}^2 = \mathbf{c}^3/3$. It follows for the second row

$$a_{21}c_1^2 + a_{22}c_2^2 = a_{22}c_2^2 = c_2^3/3$$

With the setting $a_{21} = a_{22}$ we get $a_{22} = 0$ or $c_2 = 0$. $\square$

Runge-Kutta methods have the advantage that they allow an easy implementation and automatic steplength control. Let us suppose that our Runge-Kutta method has order p. A second method with the coefficients a_{ij}, $\hat{b}_i$ and c_i should have order $p - 1$ or $p + 1$ and give the numerical solution

$$\hat{\mathbf{u}}_{m+1} = \mathbf{u}_m + \sum_{i=1}^{s} \hat{b}_i \mathbf{k}_i.$$

The new steplength τ_{m+1} can be suggested by help of the two approximations u_{m+1} and $\hat{u}_{m+1}$, i.e.

$$\tau_{m+1} = \frac{\tau_m^2}{\tau_{m-1}} \left(\frac{TOL \cdot r_n}{r_{n+1}^2} \right)^{1/p},$$

where TOL is a given tolerance and

$$r_{n+1} := \|\mathbf{u}_{m+1} - \hat{\mathbf{u}}_{m+1}\|.$$

It is possible to use a safety factor ρ. This step size selection rule is called PI-controller and due to Gustafsson et. al. [10]. More informations about the numerical error and the implementation of automatic steplength control can be found in [11, 21]. Under the expression a pair of Runge-Kutta methods with order $(p, p-1)$ we mean that the original RK method has order p and the embedded method has order $p-1$.

Next we consider a DAE of index 2

$$\dot{\mathbf{u}} = \mathbf{F}(t, \mathbf{u}, \mathbf{p}) \tag{13}$$

$$0 = \mathbf{G}(\mathbf{u}), \tag{14}$$

where the matrix product $\frac{\partial G}{\partial \mathbf{u}} \frac{\partial F_p}{\partial \mathbf{v}}$ is regular. We assume furthermore that some consistent initial conditions are given. We want to solve the DAE (13)-(14) by the help of a Runge-Kutta method. Therefore we rewrite (11) in the form

$$\mathbf{u}_{m+1} = \mathbf{u}_m + \sum_{i=1}^{s} b_i \mathbf{k}_i, \quad \mathbf{p}_{m+1} = \mathbf{p}_m + \sum_{i=1}^{s} b_i \mathbf{l}_i \tag{15}$$

$$\mathbf{k}_i = \tau \mathbf{F}(t_m + c_i\tau, \mathbf{U}_i, \mathbf{P}_i), \quad \mathbf{l}_i = \tau \mathbf{G}(t_m + c_i\tau, \mathbf{U}_i) \tag{16}$$

$$\mathbf{U}_i = \mathbf{u}_m + \sum_{j=1}^{s} a_{ij} \mathbf{k}_j, \quad \mathbf{P}_i = \mathbf{p}_m + \sum_{j=1}^{s} a_{ij} \mathbf{l}_j. \tag{17}$$

Note, that in the case that the coefficient matrix A is singular, the values l_j in (15)-(17) are not well-defined. But it is sufficient to solve an equivalent system. For more details the interested reader is refered to the paper of Jay [13].

Next we present a convergence result for the DAE (15)-(17).

Theorem 2.4 *Consider the DAE* (13)-(14) *and the Runge-Kutta method* (15)-(17). *Assume that the coefficients of the RK method satisfy the conditions $B(p)$, $C(q)$, and $D(r)$, and that the hypotheses $(H1)-(H4)$ hold. Moreover the RK method should be strongly A-stable and we suppose that the initial conditions are consistent, i.e.* $\mathbf{u}_0$ *and* $\mathbf{p}_0$ *satisfy* (13)-(14).

Let $t_m - t_0 \leq m\tau \leq$ const. Then the global error satisfies

$$\mathbf{u}_m - \mathbf{u}(t_m) = \mathcal{O}(\tau^{\min\{p,2q,q+r+1\}}), \tag{18}$$
$$\mathbf{p}_m - \mathbf{p}(t_m) = \mathcal{O}(\tau^q). \tag{19}$$

Proof see [13]. □

Lemma 3 *Let a RK method satisfying $(H1) - (H4)$ be given. Then $r = 0$ holds.*

Proof Consider the condition $D(1)$ for $j = s$ and $k = 1$. We have

$$\sum_{i=1}^{s} b_i a_{is} = b_s a_{ss} = a_{ss}^2 \neq b_s(1 - c_s) = 0.$$

□

Lemma 4 *Suppose that an RK method satisfying $(H1) - (H4)$, $B(p)$, and $C(q)$ is given. Consider the DAE* (13)-(14). *Then the global error satisfies at least*

$$\mathbf{u}_m - \mathbf{u}(t_m) = \mathcal{O}(\tau^3),$$

Proof From Lemma 3 we know that $r = 0$. Moreover $q \leq 2$ holds. Using the results of Theorem 2.4 the assertion follows. □

3 Methods with three internal stages

Our new methods should have consistency order $p = 2, 3$, stage order $q = 2$ and be strongly A-stable, i.e. the following conditions should be satisfied

$$\begin{array}{lrl} B(1): & \mathbf{b}^\top\mathbf{e} & = 1, \\ B(2): & \mathbf{b}^\top\mathbf{c} & = 1/2, \\ B(3): & \mathbf{b}^\top\mathbf{c} & = 1/3, \\ C(1): & A\mathbf{e} & = \mathbf{c}, \\ C(2): & A\mathbf{c} & = \mathbf{c}^2/2. \end{array} \tag{20}$$

With these setting it is impossible to construct a stiffly accurate DIRK method whose embedded method is again stiffly accurate.

Lemma 5 *Consider the Runge-Kutta-method with the following Butcher-table*

$$\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
1 & 1-a_{22} & a_{22} & 0 \\
1 & 1-a_{32}-a_{33} & a_{32} & a_{33} \\
\hline
 & 1-a_{32}-a_{33} & a_{32} & a_{33} \\
\hline
 & 1-a_{22} & a_{22} & 0
\end{array}$$

There exists no pair of Runge-Kutta methods with order (3,2) which satisfies $B(2)$, $B(3)$, and $C(2)$.

Proof Using $B(2)$ and $B(3)$ we have

$$\begin{aligned} b_2 + b_3 &= 1/2 \\ b_2 + b_3 &= 1/3. \end{aligned}$$

But this system has no solution. □

Lemma 6 *Consider again the Runge-Kutta-method with the following Butcher-table*

$$\begin{array}{c|ccc}
0 & 0 & 0 & 0 \\
1 & 1-a_{22} & a_{22} & 0 \\
1 & 1-a_{32}-a_{33} & a_{32} & a_{33} \\
\hline
 & 1-a_{32}-a_{33} & a_{32} & a_{33} \\
\hline
 & 1-a_{22} & a_{22} & 0
\end{array}$$

There exists no pair of Runge-Kutta methods with order (2,1) which satisfies $B(2)$ and $C(2)$.

Proof The embedded method should have only order 1, i.e.

$$\hat{\mathbf{b}}^\top \mathbf{c} \neq 1/2.$$

But with the setting $\hat{b}_1 = \hat{b}_2 = 1/2$ it follows

$$\hat{\mathbf{b}}^\top \mathbf{c} = 1/2.$$

This is a contradiction. □

These two lemmata show that it is only possible to consider DIRK methods whose embedded method is not stiffly accurate. But these methods can only be strongly A-stable and not L-stable.

Lemma 7 *There exists no L-stable DIRK method which satisfies $B(1)$, $B(2)$, $B(3)$, and $C(2)$.*

Proof The condition for L-stability implies

$$2a_{32} + a_{33} = 2b_2 + b_3 = 1. \tag{21}$$

Together with $B(2)$ and $B(3)$ we have a non-linear system for a_{22}, b_2 and b_3, i.e.

$$b_1c_1 + b_2c_2 + b_3c_3 = 2a_{22}b_2 + b_3 = 1/2 \tag{22}$$
$$b_1c_1^2 + b_2c_2^2 + b_3c_3^2 = 4a_{22}^2b_2 + b_3 = 1/3 \tag{23}$$
$$2a_{32} + a_{33} = 2b_2 + b_3 = 1. \tag{24}$$

Inserting (24) into (22) and (23) yields

$$\begin{aligned} 2(a_{22} - 1)b_2 + &= -1/2 \\ 2(2a_{22}^2 - 1)b_2 &= -2/3. \end{aligned}$$

It follows with a short calculation that

$$6a_{22}^2 - 4a_{22} + 1 = 0$$

holds. But this quadratic equation has the complex solution

$$a_{22} = \frac{1}{3} \pm \frac{i}{6}\sqrt{2}.$$

Hence the system (22)-(24) has no real solution and there exists no DIRK method satisfying all conditions stated above. □

Note, that for DIRK methods stiffly accurate and L-stability are not equivalent. This equivalence is only true if the matrix A of the Runge-Kutta method is regular.

3.1 A third order method with 3 internal stages

We have seen in the last section that the embedded method can not be stiffly accurate and that the DIRK method is only strongly A-stable. Next we start with the Butcher-table

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 2a_{22} & a_{22} & a_{22} & 0 \\ 1 & 1 - a_{32} - a_{33} & a_{32} & a_{33} \\ \hline & 1 - a_{32} - a_{33} & a_{32} & a_{33} \\ \hline & 1 - \hat{b}_2 - \hat{b}_3 & \hat{b}_2 & \hat{b}_3 \end{array}.$$

This method satisfies $B(1)$ and $C(1)$. Moreover $B(2)$ and $C(2)$ are equivalent. The three coefficients a_{22}, a_{32}, and a_{33} should fulfill the conditions $B(2)$ and $B(3)$. We get the system

$$\begin{aligned} b_1c_1 + b_2c_2 + b_3c_3 &= 2a_{22}b_2 + b_3 = 2a_{22}a_{32} + a_{33} = 1/2 \\ b_1c_1^2 + b_2c_2^2 + b_3c_3^2 &= 4a_{22}^2b_2 + b_3 = 4a_{22}^2a_{32} + a_{33} = 1/3. \end{aligned}$$

It follows immediately that

$$a_{32} = -\frac{1}{12a_{22}(2a_{22}-1)},$$
$$a_{33} = \frac{3a_{22}-1}{3(2a_{22}-1)}.$$

The coefficent a_{22} is a free variable and can be chossen arbritarely. Moreover $R(\infty)$ is given by

$$R(\infty) = \frac{6a_{22}^2 - 4a_{22} + 1}{2(3a_{22}-1)a_{22}}.$$

A first choice is $a_{22} = a_{33}$. In this case the coeffient matrices of the simplified Newton-iterations are equal. We get for a_{22} the non-linear equation

$$a_{22} = \frac{3a_{22}-1}{3(2a_{22}-1)}$$

which has the solutions

$$a_{22} = \frac{1}{2} \pm \frac{\sqrt{3}}{6}.$$

The solution $a_{22} = \frac{1}{2} - \frac{\sqrt{3}}{6}$ implies $R(\infty) = 1 + \sqrt{3}$, but this method would not be A-stable. The other solution implies $R(\infty) = \sqrt{3} - 1 \approx 0.73$.

Next we look for an embedded method of order 1. This scheme should be of order 1 and be L-stable. A short calculation using a formal manipulation program, i.e. MAPLE, yields

$$\hat{b}_1 = \frac{5}{12} + \frac{\sqrt{3}}{12},$$
$$\hat{b}_2 = \frac{3}{4} + \frac{\sqrt{3}}{12},$$
$$\hat{b}_3 = -\frac{1}{6} - \frac{\sqrt{3}}{6}.$$

We call this method DIRK3. If one looks for the minimum of $R(\infty)$ with respect to a_{22} then one obtains again our new method DIRK3.

3.2 An L-stable method of order 2 with 3 internal stages

We have seen at the beginning of this section that an L-stable method can not be of order 3. Therefore we look in this section for an L-stable method of order 2.

Again, we start with the Butcher-table

$$\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 2a_{22} & a_{22} & a_{22} & 0 \\ 1 & 1-a_{32}-a_{33} & a_{32} & a_{33} \\ \hline & 1-a_{32}-a_{33} & a_{32} & a_{33} \\ \hline & 1-\hat{b}_2-\hat{b}_3 & \hat{b}_2 & \hat{b}_3 \end{array}$$

The conditions $B(1)$ and $C(1)$ are satisfied and the conditions $B(2)$ and $C(2)$ are equivalent. The three coefficients a_{22}, a_{32}, and a_{33} should fulfill the condition $B(2)$ and the condition for the L-stability, i.e. equation (21). We get the system

$$\begin{aligned} 2a_{22}b_2 + b_3 &= 1/2 \\ 2b_2 + b_3 &= 1. \end{aligned}$$

Subtracting both equations we obtain

$$2(1-a_{22})b_2 = 1/2$$

and finally

$$b_2 = \frac{1}{4(1-a_{22})}, \qquad b_3 = \frac{1-2a_{22}}{2(1-a_{22})}.$$

The setting $a_{22} = a_{33}$ implies

$$2a_{22}^2 - 4a_{22} + 1 = 0.$$

This equation have the solutions $a_{22} = 1 \pm \frac{\sqrt{2}}{2}$. Since $1 + \frac{\sqrt{2}}{2} > 1$ we choose the second solution $a_{22} = 1 - \frac{\sqrt{2}}{2}$.

Finally we look for an embeded method which should be of order 1. This method can not be L-stable since this method is then of order 2. Therefore we set $\hat{R}(\infty) = 1/2$. Then the coefficients of our embedded method are given by

$$\hat{b}_1 = \hat{b}_2 = \frac{1}{2} - \frac{1}{8}\sqrt{2}, \qquad \hat{b}_3 = \frac{1}{4}\sqrt{2}.$$

We call our new method DIRK3L, where L stands for L-stable. Moreover the scheme DIRK3L can be obtained, too, if the problem $|\sum b_i c_i^2 - 1/3| \to \min!$ is solved.

4 Methods with four internal stages

We have shown in the last section that a stiffly accurate DIRK method whose embedded method is stiffly accurate, too, should have four or more internal stages. Solving the incompressible Navier-Stokes equations with automatic stepsize selection and embedding, it is advantageous to use an stiffly accurate embedded method.

4.1 A third order method with four internal stages

Our new method should have consistency order $p = 3$, stage order $q = 2$ and be L-stable, i.e. the following conditions should be satisfied

$$\begin{array}{rrl} B(1): & \mathbf{b}^\top \mathbf{e} & = 1, \\ B(2): & \mathbf{b}^\top \mathbf{c} & = 1/2, \\ B(3): & \mathbf{b}^\top \mathbf{c} & = 1/3, \\ C(1): & A\mathbf{e} & = \mathbf{c}, \\ C(2): & A\mathbf{c} & = \mathbf{c}^2/2, \\ L: & a_{33} - a_{43} - a_{33}a_{44} + 2a_{32}a_{43} - 2a_{42}a_{33} & = 0. \end{array}$$

We consider the DIRK method with the following Butcher-table

$$\begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 2a_{22} & a_{22} & a_{22} & 0 & 0 \\ 1 & 1 - a_{32} - a_{33} & a_{32} & a_{33} & 0 \\ 1 & 1 - a_{42} - a_{43} - a_{44} & a_{42} & a_{43} & a_{44} \\ \hline & 1 - a_{42} - a_{43} - a_{44} & a_{42} & a_{43} & a_{44} \\ \hline & 1 - a_{32} - a_{33} & a_{32} & a_{33} & 0 \end{array}$$

Again the property stiffly accurate does not imply L-stability.

Lemma 8 *There exists no pair of DIRK methods with order (3,2) satisfying* $(H1) - (H4)$ *and whose embedded method is stiffly accurate and L-stable, too.*

Proof First we consider the condition of the L-stability of the embedded method. We have

$$\hat{R}(\infty) = \frac{a_{33} + 2a_{32} - 1}{a_{33}}.$$

Together with $\hat{B}(2)$, $C(2)$ and the condition for the L-stability we have the system

$$\begin{array}{rrl} B(2): & 2a_{22}b_2 + b_3 + b_4 & = 1/2 \\ B(3): & 4a_{22}^2 b_2 + b_3 + b_4 & = 1/3 \\ \hat{B}(2): & 2a_{32}a_{22} + a_{33} & = 1/2 \\ \hat{R}(\infty): & 2a_{32} + a_{33} & = 1 \\ R(\infty): & a_{33}(1 - 2b_2) + (2a_{32} - 1)b_3 - a_{33}b_4 & = 0. \end{array}$$

The conditions $B(2)$ and $B(3)$ imply

$$2a_{22}(2a_{22}-1)b_2 = -1/6.$$

Next the terms $\hat{B}(2)$ and $\hat{R}(\infty)$ can be used to obtain

$$2a_{32}(a_{22}-1) = -1/2.$$

All these equations are used to simplify $R(\infty)$. We get

$$\begin{aligned}
0 &= a_{33}(1-2b_2) + (2a_{32}-1)b_3 - a_{33}b_4 \\
&= (1-2a_{32})(1-2b_2) + (2a_{32}-1)b_3 - (1-2a_{32})b_4 \\
&= (1-2a_{32})(1-2b_2-b_3-b_4) \\
&= (1-2a_{32})(1-2b_2+2a_{22}b_2-1/2) \\
&= \frac{1}{2}(1-2a_{32})(1+4(a_{22}-1)b_2).
\end{aligned}$$

To obtain a solution of the last equation one of the factors $1-2a_{32}$ and $1+4(a_{22}-1)b_2$ should be 0. If the first factor is equal zero, then it follows $a_{32}=1/2$. But this implies with $\hat{R}(\infty)$ that $a_{33}=0$. Hence $1+4(a_{22}-1)b_2=0$ or $4(1-a_{22})b_2=1$. It follows

$$4(1-a_{22})b_2 = 4(1-a_{22})\frac{-1}{12a_{22}(2a_{22}-1)} = 1$$

and

$$a_{22}-1 = 3a_{22}(2a_{22}-1) = 6a_{22}^2 - 3a_{22}.$$

The solutions are complex and given by

$$a_{22} = \frac{1}{3} \pm \frac{i}{\sqrt{18}}.$$

Hence the above scheme does not exists. $\square$

Let us suppose that our new method should satisfy the following conditions

$$\begin{array}{rrl}
B(2): & 2a_{22}b_2 + b_3 + b_4 & = 1/2 \\
B(3): & 4a_{22}^2b_2 + b_3 + b_4 & = 1/3 \\
\hat{B}(2): & 2a_{32}a_{22} + a_{33} & = 1/2 \\
R(\infty): & a_{33}(1-2b_2) + (2a_{32}-1)b_3 - a_{33}b_4 & = 0 \\
: & a_{22} = a_{33} = a_{44} & = b_4.
\end{array}$$

Using the last condition we get for the other expressions

$$\begin{array}{rrl}
B(2): & 2a_{22}b_2 + b_3 + b_4 & = 1/2 \\
B(3): & 4a_{22}^2b_2 + b_3 + b_4 & = 1/3 \\
\hat{B}(2): & 2a_{32}a_{22} + b_4 & = 1/2 \\
R(\infty): & b_4(1-2b_2-b_4) + (2a_{32}-1)b_3 & = 0
\end{array}$$

Using a formel manipulation program (for example MAPLE) we obatin a unique solution of the above the system. We coefficent of our new method DIRK34L are presendted in Table 4.

Table 4: Coefficients of the method DIRK34L

$a_{21} = 1.558983899988677E-01$	$a_{32} = 1.072486270734370E+00$
$a_{42} = 7.685298292769537E-01$	$a_{43} = 9.666483609791597E-02$

4.2 A fourth order method with four internal stages

Next we want to derive a method with $p = 4$. Since the method DIRK34L does not satisfiy $B(3)$ we cannot expect that $a_{22} = a_{33} = a_{44}$. We have to solve the following non-linear system

$$\begin{array}{lrl} B(2): & 2a_{22}b_2 + b_3 + b_4 & = 1/2 \\ B(3): & 4a_{22}^2 b_2 + b_3 + b_4 & = 1/3 \\ B(4): & 8a_{22}^3 b_2 + b_3 + b_4 & = 1/4 \\ \hat{B}(2): & 2a_{32}a_{22} + a_{33} & = 1/2 \\ R(\infty): & a_{33}(1-2b_2) + (2a_{32}-1)b_3 - a_{33}b_4 & = 0. \end{array}$$

Using MAPLE we get a solution which depends on a_{44}

$$\begin{aligned} a_{21} &= a_{22} = 1/4, \\ a_{32} &= \frac{3a_{44}-2}{3(3a_{44}-1)}, \\ a_{33} &= \frac{6a_{44}-1}{6(3a_{44}-1)}, \\ a_{42} &= \frac{2}{3}, a_{43} = \frac{1}{6} - a_{44}. \end{aligned}$$

The coefficient a_{44} can be choosen in such a way that

$$|R(z) - e^z| = \left| \frac{18a_{44}^2 - 6a_{44} + 1}{144(3a_{44}-1)} + \mathcal{O}(z^5) \right| \to \text{min!}$$

This leads to $a_{44} = \frac{1}{3} - \frac{\sqrt{2}}{6}$. This method is called DIRK44L.

5 Numerical example

All examples are solved numerically by the help of the FEM-package MooNMD (see [18]) on a uniform spatial grid consisting of 1024 quadrangles, i.e. $h = 2^{-5}$. We compare our new methods with other well-known methods such as the Crank-Nicolson-scheme (CN), the fractional-step-θ-method (FS) and methods from Alexander [1]. An overview of the selected methods can be found in Table 5.

The global error $\underline{\epsilon}$ is measured in the discrete L_2-norm ($\|\underline{\epsilon}\|_{l_2(N)}$), and the numerically observed temporal order of convergence is computed by

$$q_{num} = \log_2\left(\frac{\|\underline{\epsilon}\|_{l_2(N)}}{\|\underline{\epsilon}\|_{l_2(2N)}}\right).$$

The numerical results are obtained with the finite-element code MooNMD [18]

Table 5: Properties of the selected Rosenbrock methods

Name	s	p	q	$R(\infty)$	embedding	reference
CN	2	2	$\{1,2\}$	1	no	[11, 25]
FS	4	2	1	$\sqrt{2}/2$	yes	[8, 25]
Dirk3	3	3	2	$\sqrt{3}-1$	yes	3.1
Dirk3L	3	3	2	0	yes	3.2
Dirk34	4	3	2	0	yes, st. acc.	4.1
Dirk44	4	4	2	0	yes, st. acc.	4.2
Alexander (3,2)	4	4	2	0	yes	[1]
Alexander (4,3)	4	4	2	0	yes	[1]

and the numerical error ε is measured in the discrete l_2-norm

$$\|\boldsymbol{\varepsilon}\|_{l_2^{(N+1)}(0,T,X)} = \left(\frac{1}{N}\sum_{n=0}^{N}\|\mathbf{u}_n - \mathbf{u}(t_n)\|_X^2\right)^{1/2},$$

where $X = V$ and $X = Q$, resp.

Example 5.1 *Let $T = 1$ and $\Omega = (0,1)^2$. We consider the incompressible Navier-Stokes-equations* (1) *with $Re = 1$. The right-hand side $\mathbf{f}$, the initial condition $\mathbf{u}_0$ and the non-homogeneous Dirichlet boundary conditions are chosen such that*

$$\begin{aligned} u_1(x,y) &= \frac{2y^2}{1+(t-2)^2}, \\ u_2(x,y) &= xe^{-100t}, \\ p(x,y) &= (10+t)e^{-t}(x+y-1) \end{aligned}$$

is the solution of (1)*. We used a mesh consisting of squares with edge length* $h = 1/32$*.*

The mapped Q_2/P_1^{disc} *finite element discretization on quadrilateral grids is used. That means, the velocity is approximated by a continuous function which is piecewise biquadratic and the pressure by a discontinuous piecewise linear function. This pair of finite element spaces is considered currently among the best performing ones in the numerical simulation of incompressible flows, see [9, 17, 14]. Note that for any* t *the solution can be represented exactly by the finite element functions. Hence, all occurring errors will result from the temporal discretization.*

In the temporal discretization, a uniform time step $\tau_n = \tau$ *for all* n *is used. The linear systems are solved with a preconditioned flexible GMRES method [27]. The preconditioner is a coupled multigrid method with Vanka smoother which is described in detail in [17, 14, 15].*

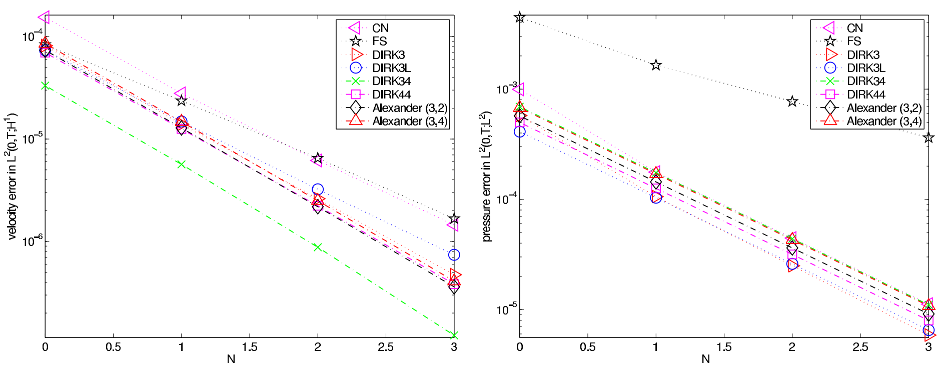

Figure 1: Results

In Figure 1 we present the numerical results. We compare all schemes presented in Table 5. The problem is solved with constant time step sizes $\tau = \frac{1}{10 \cdot 2^N}$*,* $N = 0, \ldots, 3$*.*

Considering the velocity error it can be observed that the method DIRK34L gives the best results and the Crank-Nicolson- and the fractional-step-θ*-method give the most inaccurate results since these methods are only of order 2. All other methods converge with order 3.*

If we take a look at the pressure error, we see that the fractional-step-θ *converges only linear. All other methods converge with order 2 and yield better results.*

Example 5.2 *We consider the same problem as in Example 1 and we solve the equations using automatic step length control by the help of embedding.*

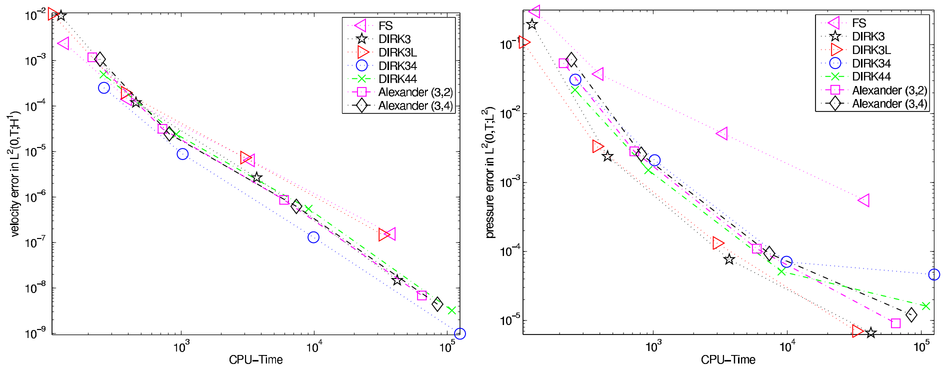

Figure 2: Results

The results are presented in Figure 2. If we look at the velocity error we observe that the fractional-step-$theta$-method and the scheme DIRK3L yield the most inaccurate results. The best results are obtained by the method DIRK34L. Considering the pressure error we get a different impression since now DIRK3 and DIRK3L yield the best results. Again the fractional-step-$theta$-method yield the most inaccurate results.

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